

**Supporting information for:**

**A QM:MM Model for the Interaction of DNA**

**Nucleotides with Carbon Nanotube**

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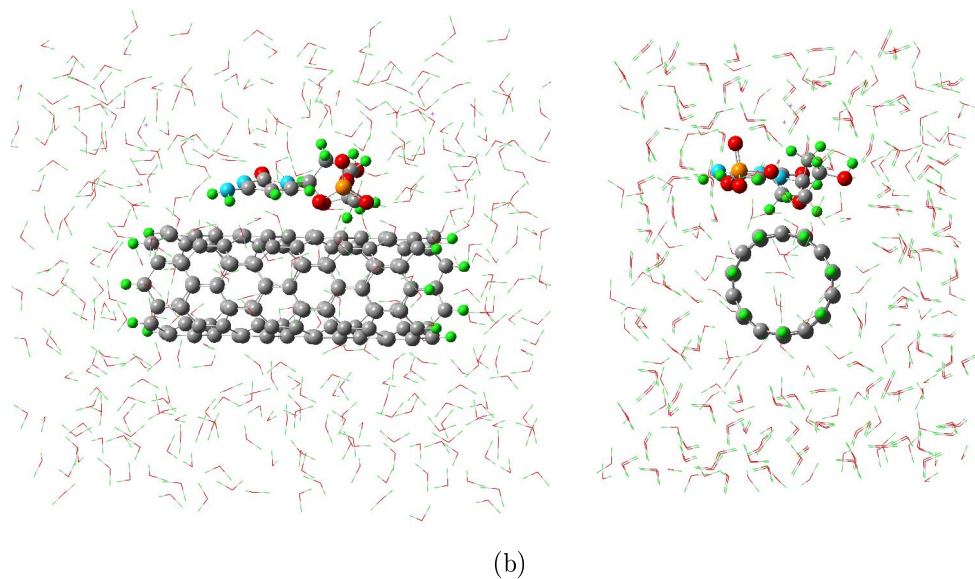
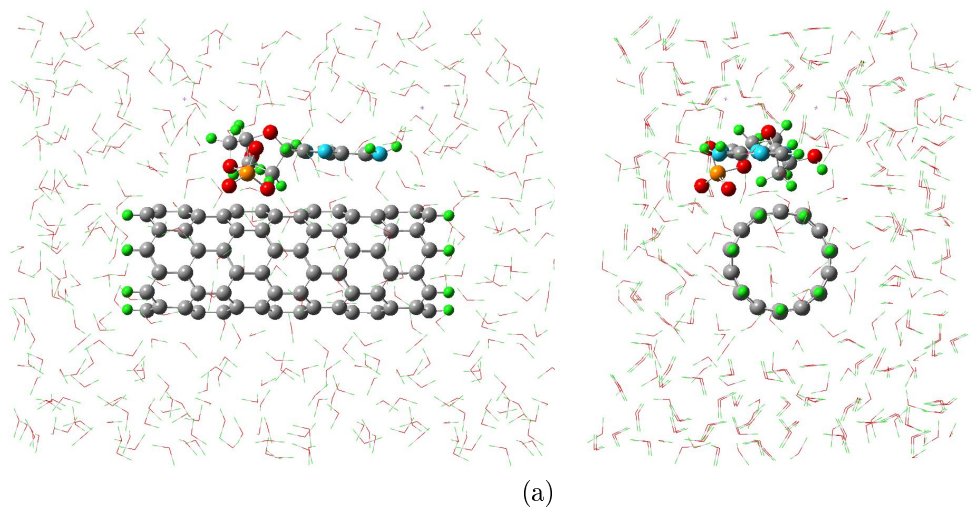


Figure S1: Initial configuration of NMP-CNT systems in solution: (a) AMP-(7,0) CNT, (b) CMP-(7,0) CNT, (c) GMP-(7,0) CNT, (d) TMP-(7,0) CNT, (e) AMP-(4,4) CNT, (f) CMP-(4,4) CNT, (g) GMP-(4,4) CNT, and (h) TMP-(4,4) CNT; left and right figures are respectively front and side view.

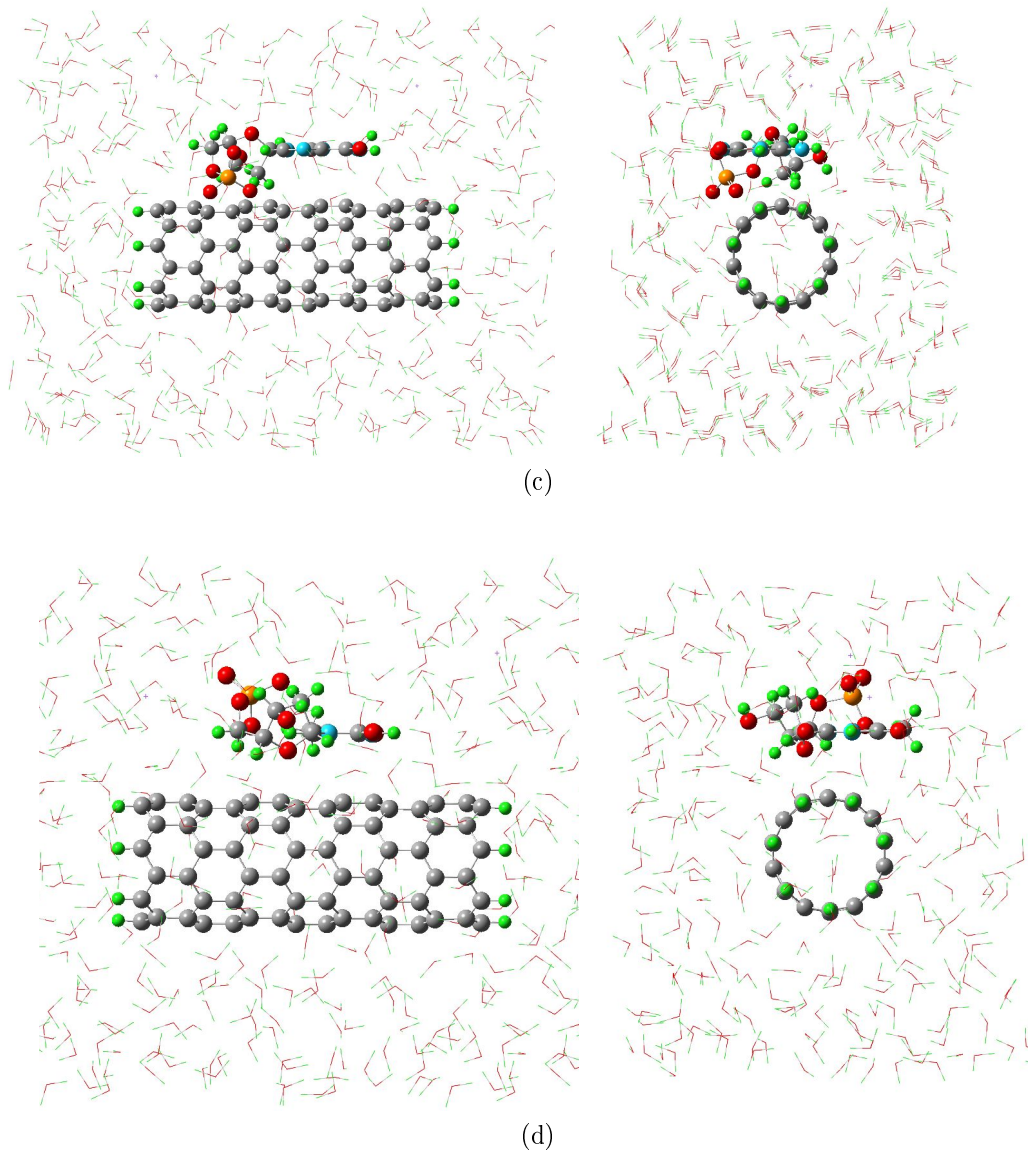


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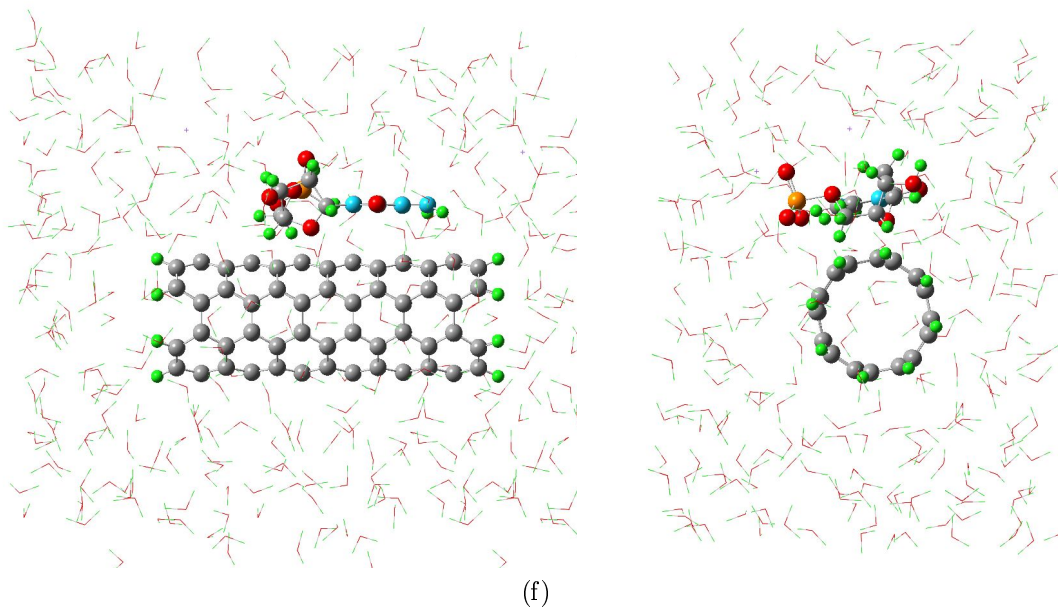
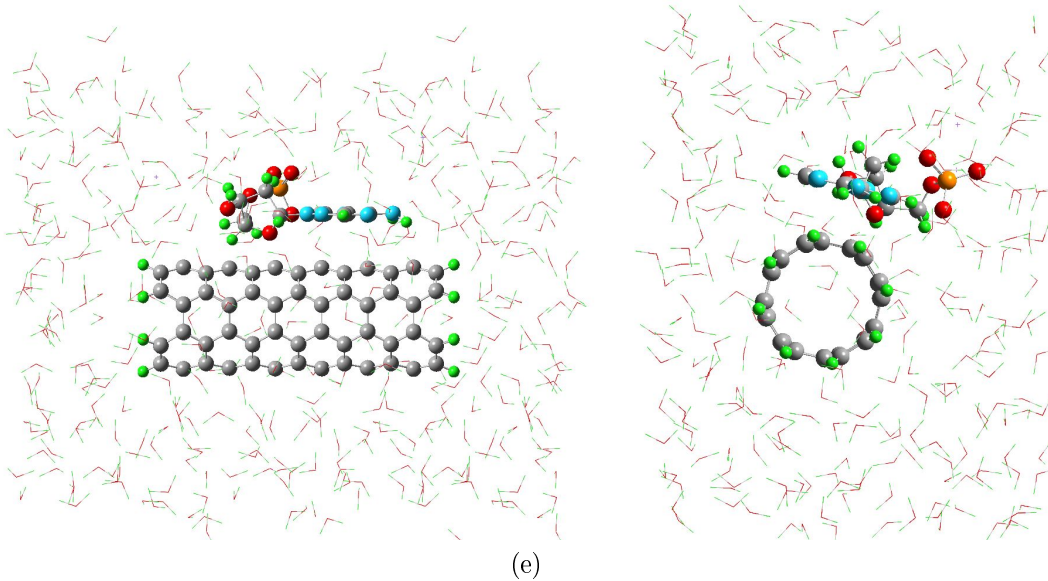


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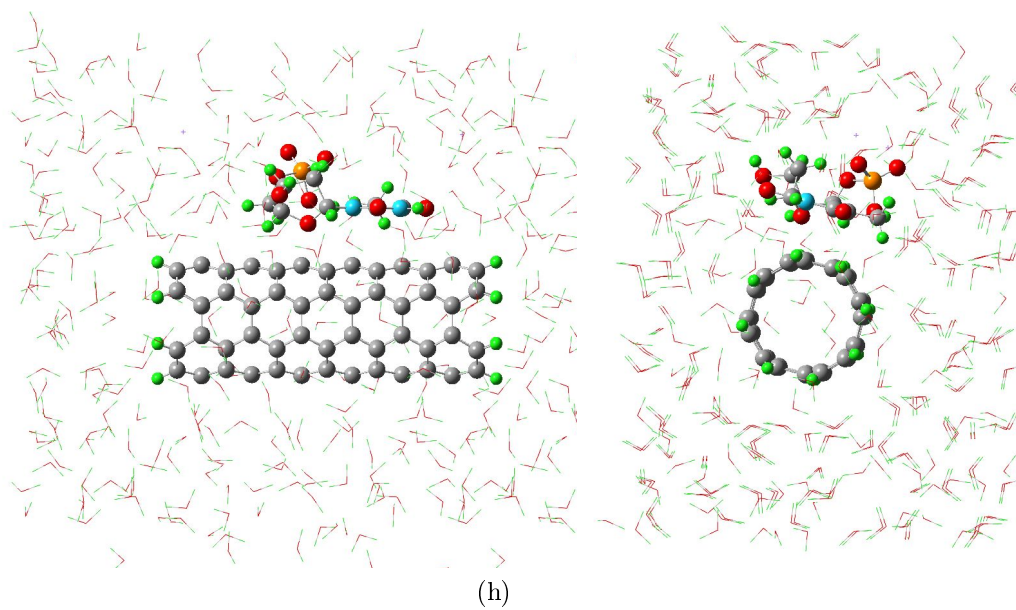
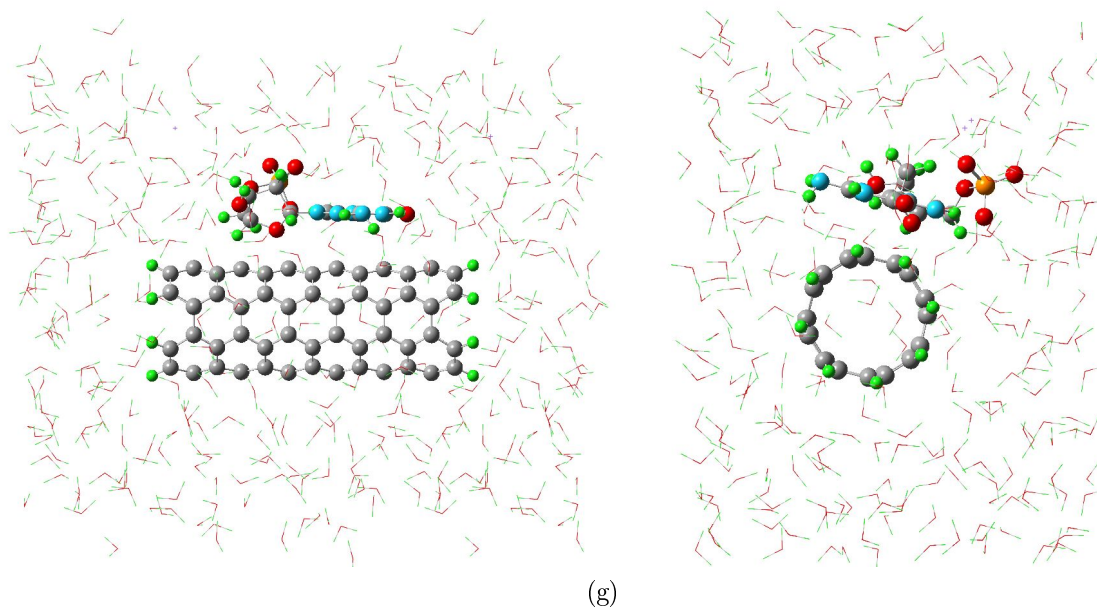


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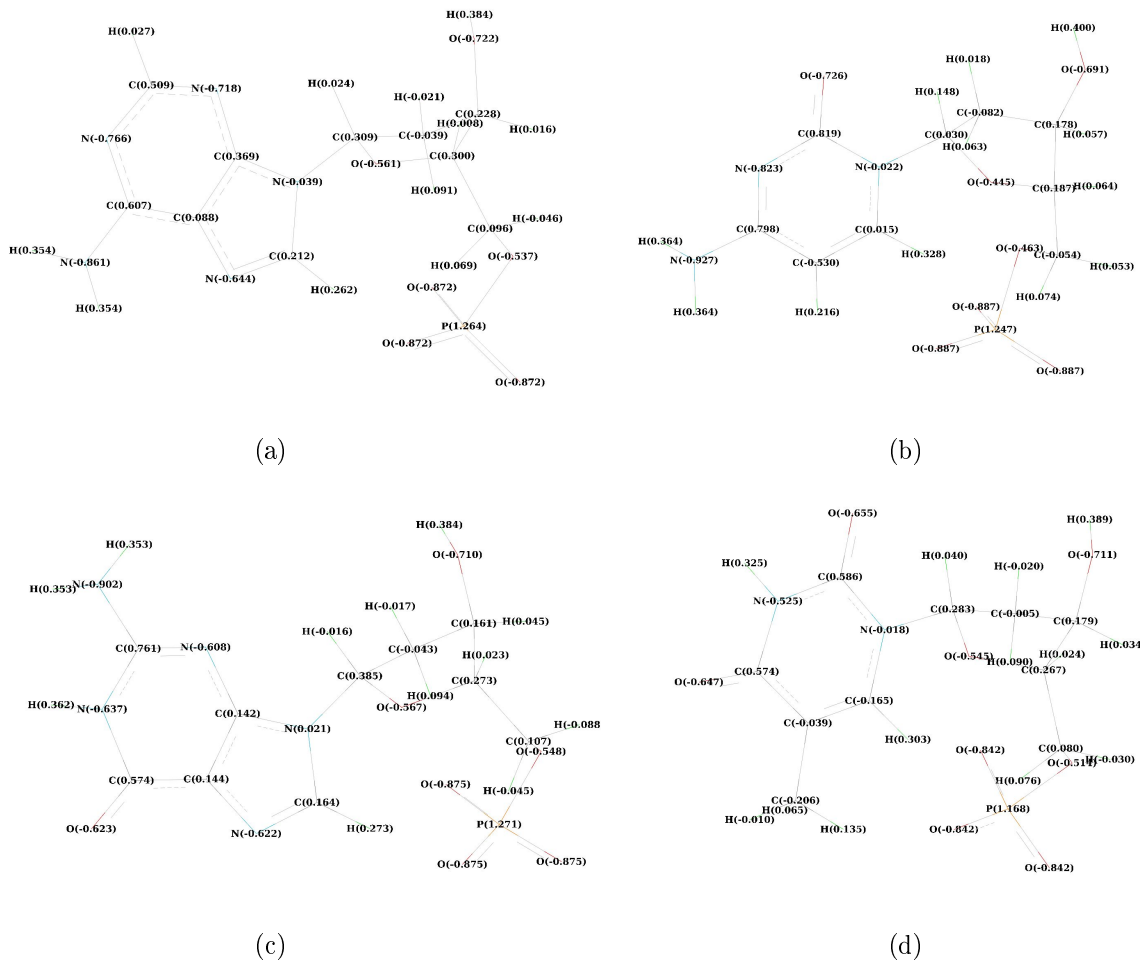
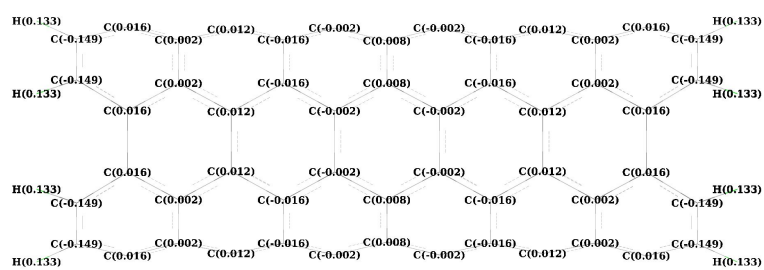
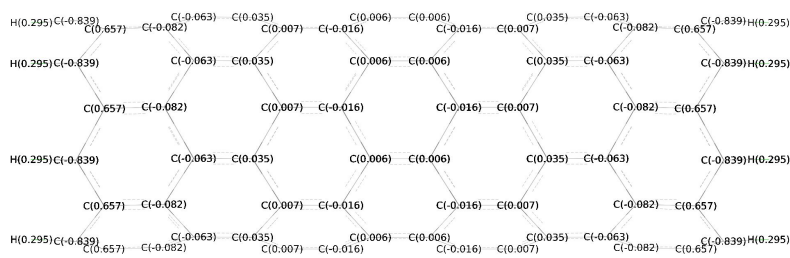


Figure S2: Atomic partial charges: (a) AMP, (b) CMP, (c) GMP, (d) TMP, (e) (4,4) CNT, and (f) (7,0) CNT.

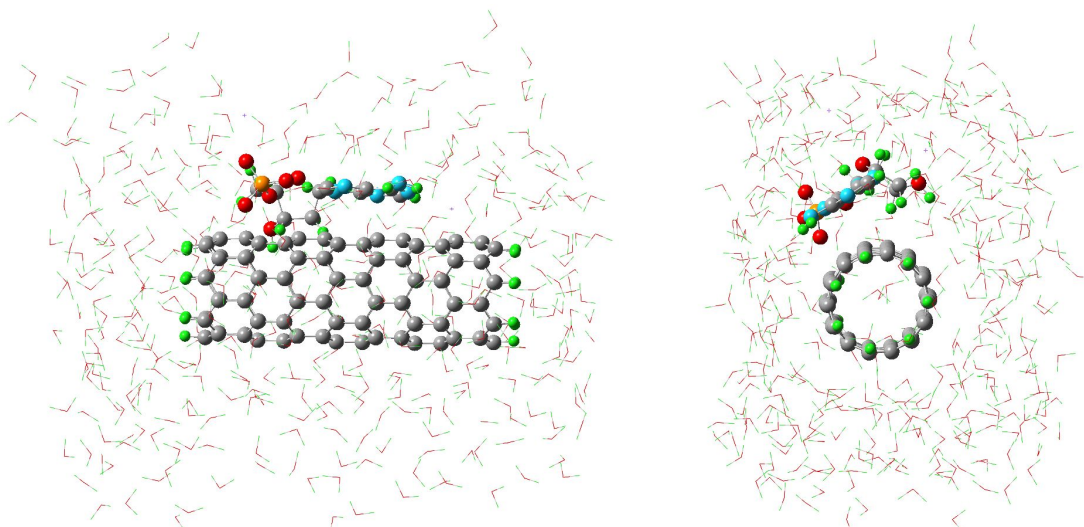


(e)

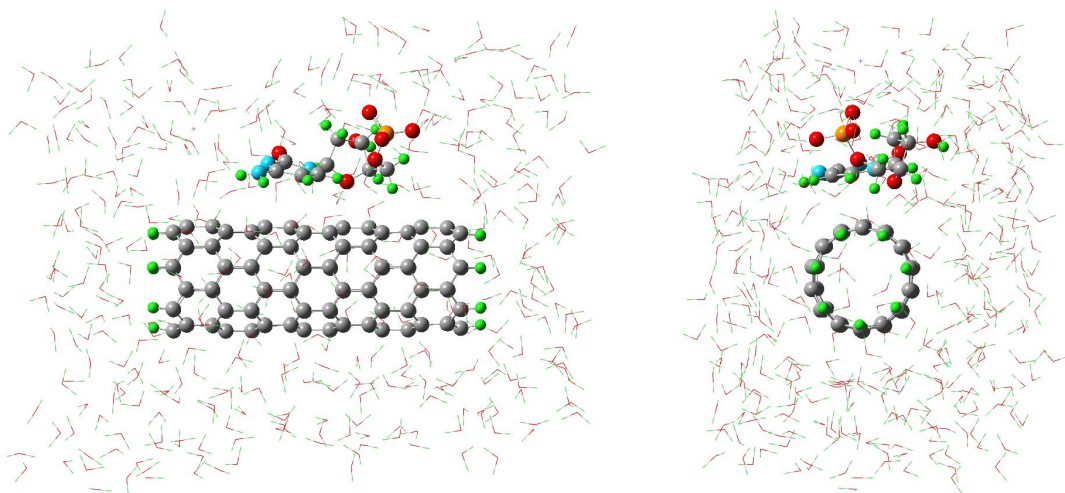


(f)

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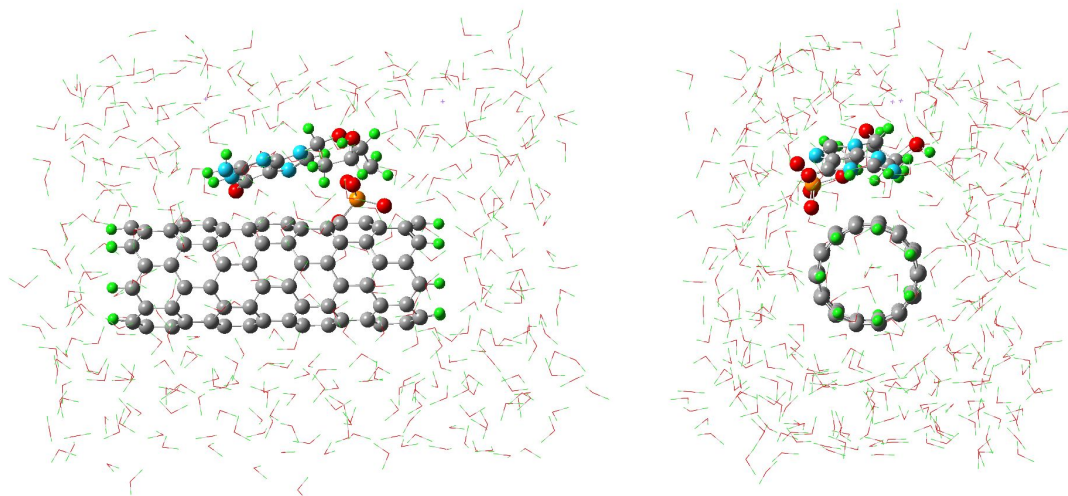
(a)



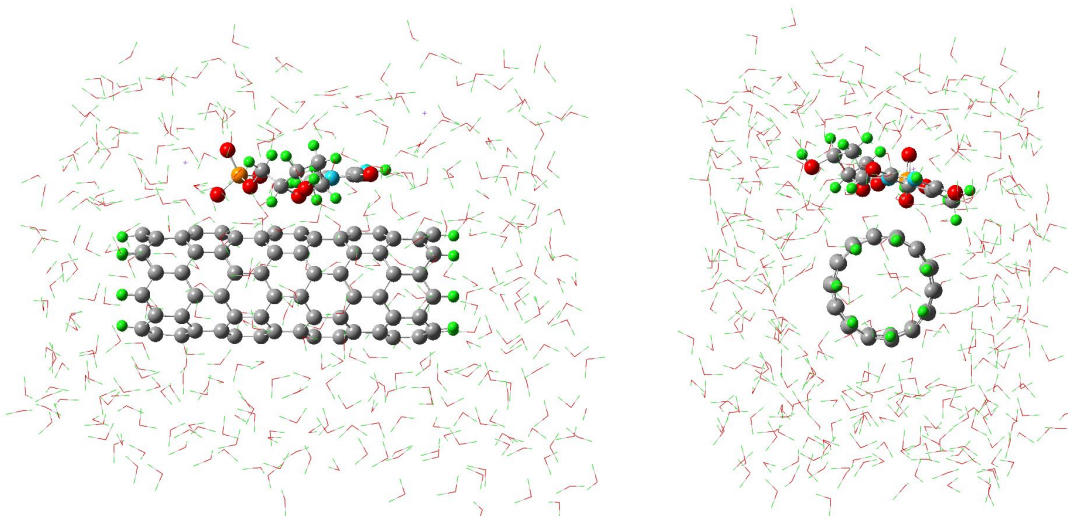
(b)

Figure S3: Final optimized configuration of NMP-CNT systems in solution: (a) AMP-(7,0) CNT, (b) CMP-(7,0) CNT, (c) GMP-(7,0) CNT, (d) TMP-(7,0) CNT, (e) AMP-(4,4) CNT, (f) CMP-(4,4) CNT, (g) GMP-(4,4) CNT, and (h) TMP-(4,4) CNT; left and right figures are respectively front and side view.



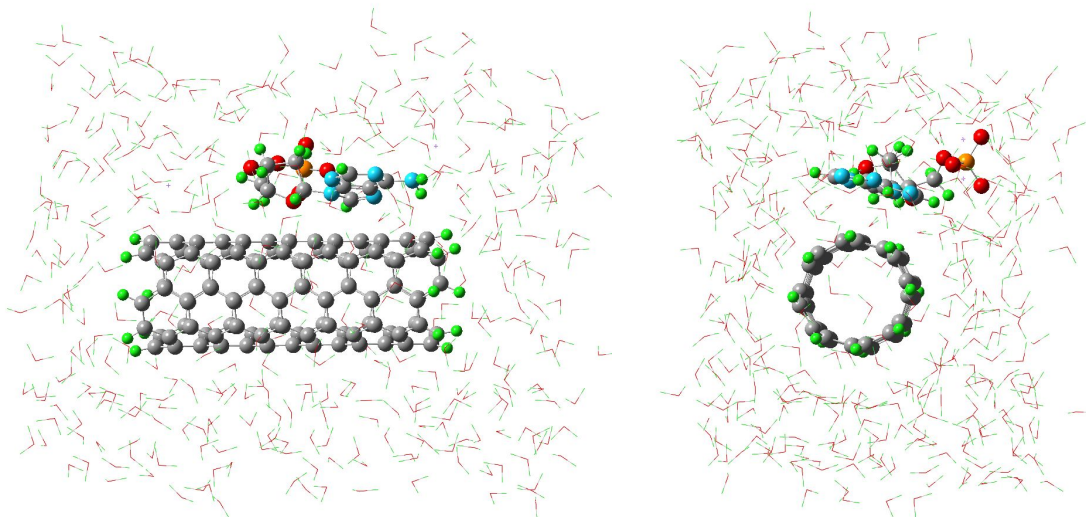


(c)

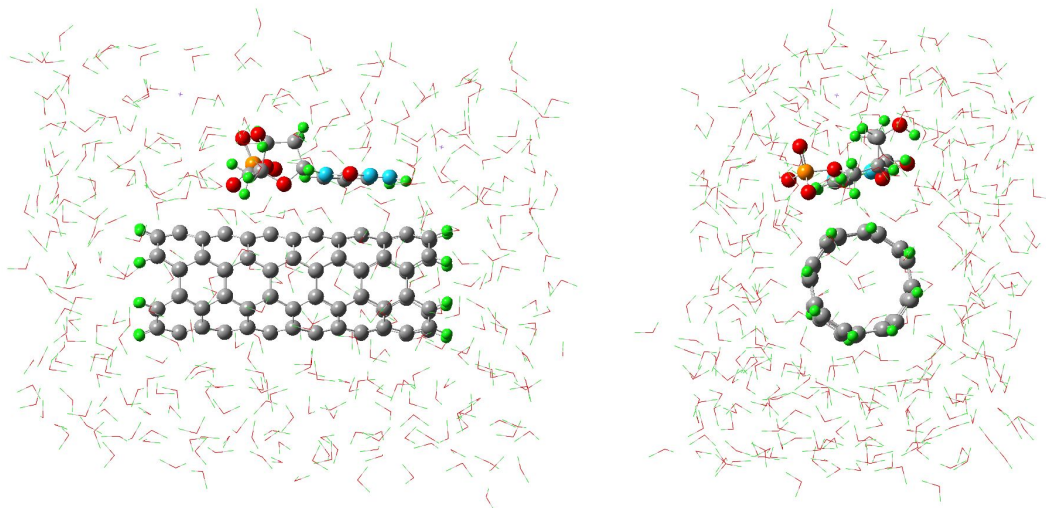


(d)

Figure S3: Final optimized configuration of NMP-CNT systems in solution: (a) AMP-(7,0) CNT, (b) CMP-(7,0) CNT, (c) GMP-(7,0) CNT, (d) TMP-(7,0) CNT, (e) AMP-(4,4) CNT, (f) CMP-(4,4) CNT, (g) GMP-(4,4) CNT, and (h) TMP-(4,4) CNT; left and right figures are respectively front and side view.

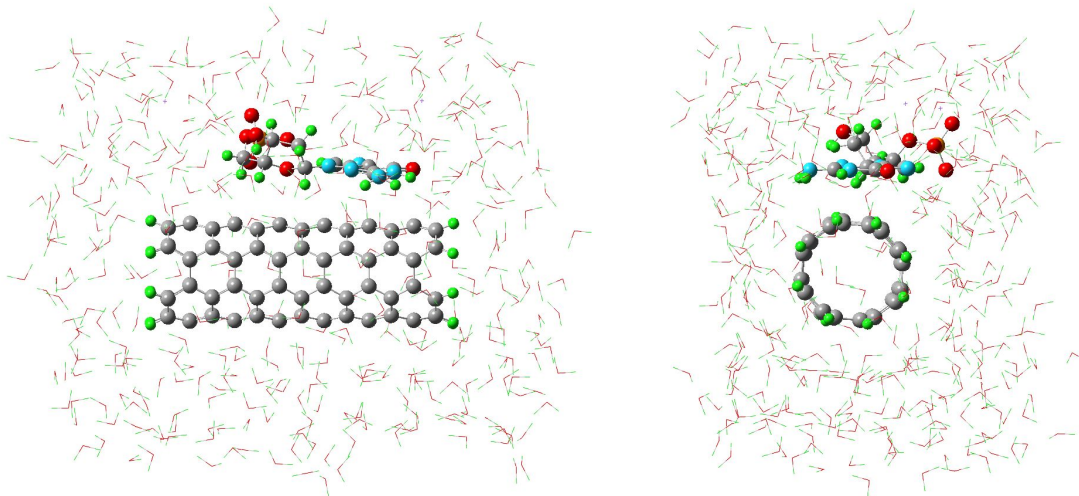


(e)

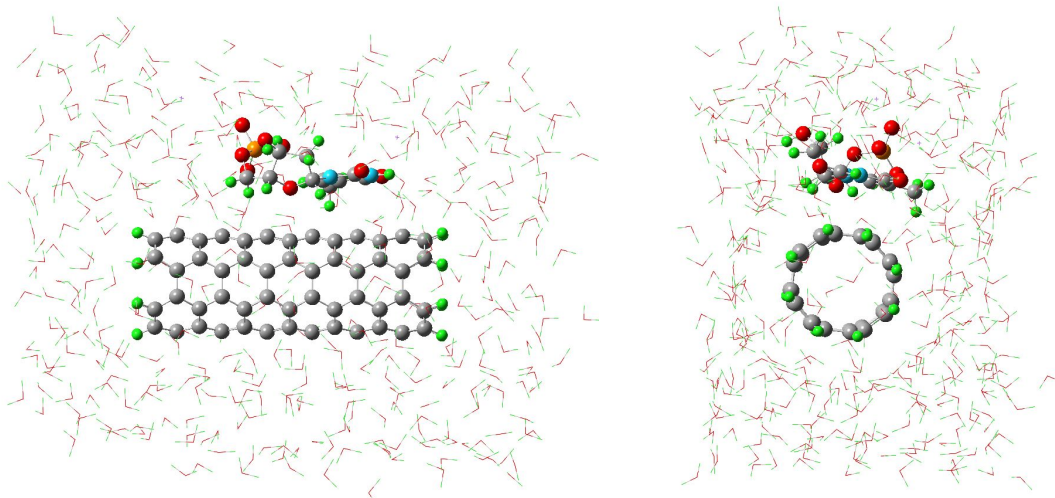


(f)

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(g)



(h)

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